



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:48 PM UTC

PDB ID : 3FRP / pdb_00003frp
Title : Crystal Structure of Cobra Venom Factor, a Co-factor for C3- and C5 convertase CVFBb
Authors : Krishnan, V.; Narayana, S.V.L.
Deposited on : 2009-01-08
Resolution : 2.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

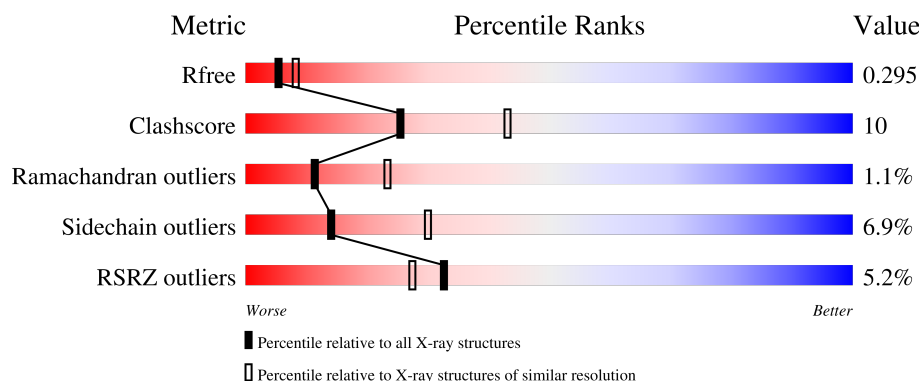
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	627	2% 73% 21% • •
2	G	252	8% 61% 21% • 15%
3	B	379	8% 65% 23% • 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9156 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cobra venom factor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4691	3009	785	882	15			

- Molecule 2 is a protein called Cobra venom factor gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	215	Total	C	N	O	S	0	0	0
			1710	1106	284	315	5			

- Molecule 3 is a protein called Cobra venom factor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	343	Total	C	N	O	S	0	0	0
			2674	1689	444	522	19			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

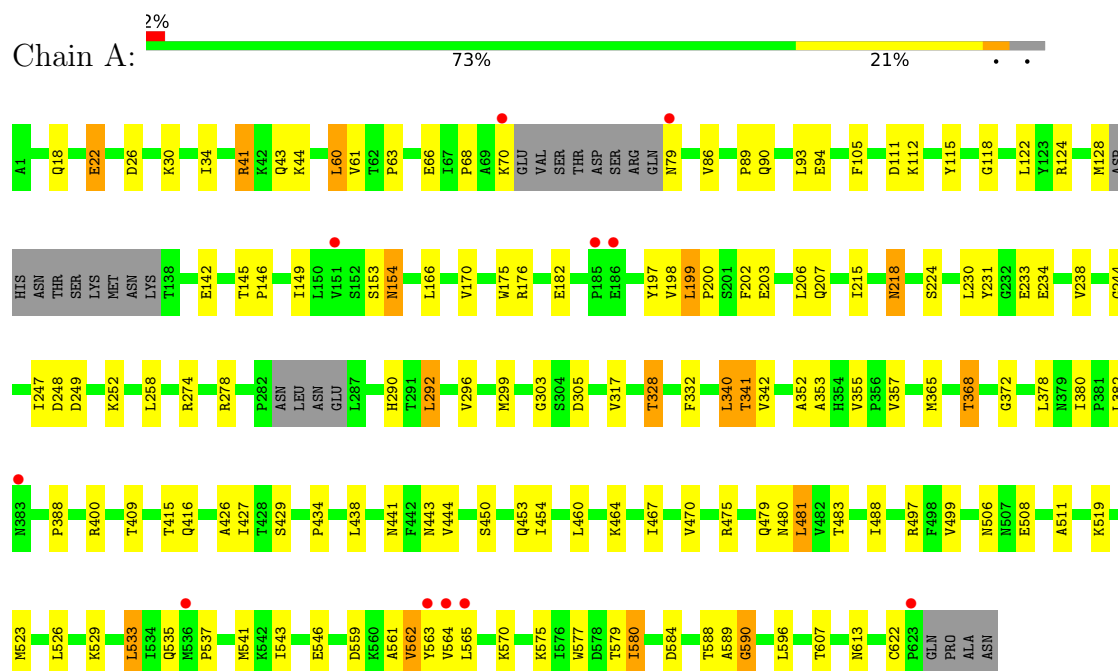
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	G	20	Total	O	0	0
			20	20		
5	B	13	Total	O	0	0
			13	13		

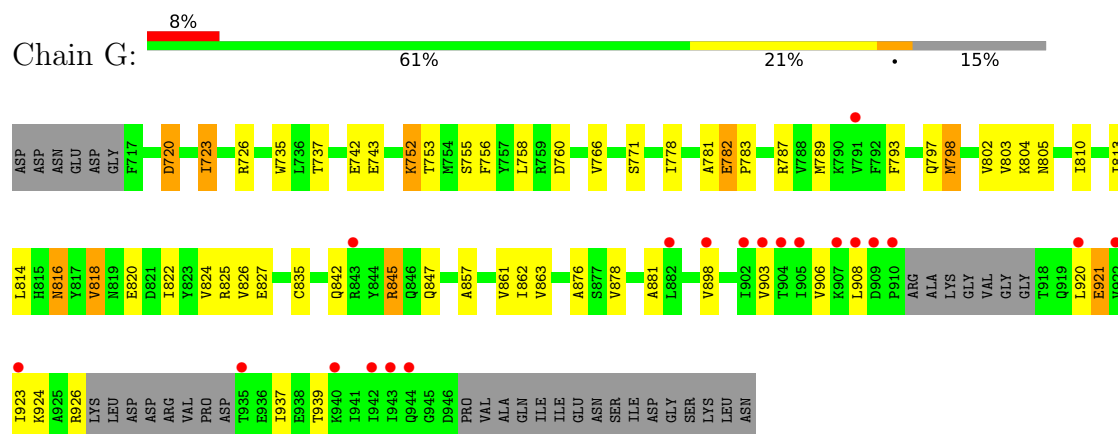
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cobra venom factor alpha chain

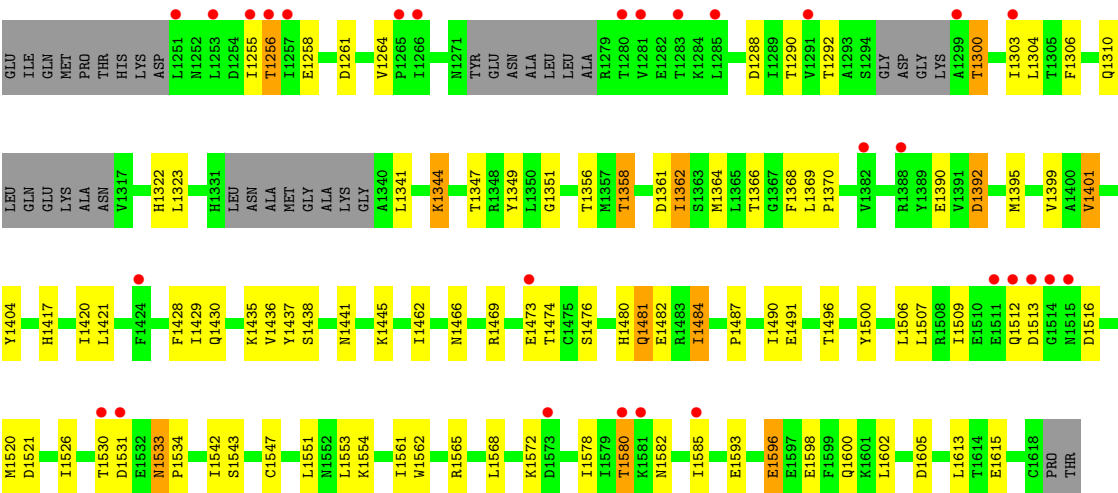


• Molecule 2: Cobra venom factor gamma chain



• Molecule 3: Cobra venom factor beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.14Å 151.14Å 76.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 50.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-2.61) 91.1 (50.00-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.248 , 0.297 0.247 , 0.295	Depositor DCC
R_{free} test set	2221 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9156	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/4797	0.90	7/6527 (0.1%)
2	G	0.71	0/1744	0.95	2/2366 (0.1%)
3	B	0.70	1/2718 (0.0%)	0.93	3/3685 (0.1%)
All	All	0.70	1/9259 (0.0%)	0.92	12/12578 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1264	VAL	CA-C	5.11	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	GLY	N-CA-C	6.46	119.60	111.85
2	G	921	GLU	N-CA-C	6.10	118.32	108.32
3	B	1533	ASN	N-CA-C	5.67	122.34	109.81
1	A	182	GLU	N-CA-C	5.44	117.64	111.11
1	A	511	ALA	N-CA-C	5.40	117.39	109.24
1	A	41	ARG	N-CA-C	5.39	117.91	111.71
1	A	622	CYS	N-CA-C	5.39	116.20	109.57
3	B	1476	SER	N-CA-C	5.30	116.78	109.15
3	B	1362	ILE	N-CA-C	5.25	115.47	108.11
1	A	506	ASN	N-CA-C	5.05	118.73	112.47
2	G	793	PHE	N-CA-C	5.05	116.51	108.79
1	A	202	PHE	N-CA-C	5.01	116.99	109.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4691	0	4699	94	0
2	G	1710	0	1731	38	0
3	B	2674	0	2530	59	0
4	A	1	0	0	0	0
5	A	47	0	0	5	0
5	B	13	0	0	0	0
5	G	20	0	0	0	0
All	All	9156	0	8960	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1561:ILE:HD11	3:B:1585:ILE:HD13	1.49	0.91
1:A:230:LEU:HD13	1:A:561:ALA:HB2	1.60	0.83
2:G:798:MET:HE3	2:G:810:ILE:HG21	1.63	0.80
3:B:1480:HIS:HA	3:B:1481:GLN:CB	2.17	0.75
3:B:1561:ILE:CD1	3:B:1585:ILE:HD13	2.18	0.72
1:A:460:LEU:HD23	1:A:467:ILE:HD12	1.71	0.72
1:A:328:THR:HG23	1:A:341:THR:H	1.55	0.71
3:B:1526:ILE:HG22	3:B:1613:LEU:HD22	1.72	0.71
1:A:218:ASN:HA	1:A:274:ARG:HD2	1.72	0.71
1:A:434:PRO:HA	1:A:488:ILE:HG22	1.76	0.67
2:G:923:ILE:O	3:B:1288:ASP:HA	1.95	0.67
1:A:230:LEU:CD1	1:A:561:ALA:HB2	2.23	0.67
1:A:588:THR:HG22	1:A:590:GLY:H	1.57	0.67
3:B:1366:THR:HG22	3:B:1430:GLN:H	1.61	0.66
3:B:1437:TYR:CD1	3:B:1445:LYS:HG2	2.30	0.66
1:A:607:THR:HG21	5:A:674:HOH:O	1.94	0.65
3:B:1516:ASP:HB2	3:B:1543:SER:O	1.96	0.65
1:A:203:GLU:HB3	1:A:564:VAL:HG22	1.80	0.64
3:B:1482:GLU:O	3:B:1602:LEU:HD11	1.97	0.64
1:A:352:ALA:O	1:A:368:THR:HG21	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:HB3	1:A:224:SER:HB2	1.79	0.63
3:B:1506:LEU:HD13	3:B:1520:MET:HE3	1.80	0.63
1:A:206:LEU:HD21	1:A:296:VAL:HG11	1.79	0.63
1:A:464:LYS:HG2	1:A:580:ILE:HD11	1.81	0.62
2:G:726:ARG:HB3	2:G:760:ASP:HB3	1.80	0.62
1:A:244:GLY:O	1:A:292:LEU:HD23	2.01	0.60
1:A:497:ARG:NH1	1:A:584:ASP:OD2	2.35	0.60
3:B:1580:THR:HG23	3:B:1582:ASN:H	1.67	0.60
1:A:86:VAL:HG22	1:A:93:LEU:HB2	1.84	0.60
1:A:118:GLY:HA2	1:A:166:LEU:O	2.00	0.60
1:A:305:ASP:HB3	2:G:797:GLN:HG2	1.82	0.60
1:A:575:LYS:O	1:A:579:THR:HG23	2.01	0.59
1:A:588:THR:HG21	5:A:631:HOH:O	2.02	0.59
1:A:388:PRO:HB3	1:A:409:THR:HG22	1.85	0.57
1:A:563:TYR:CE2	2:G:766:VAL:HG21	2.39	0.57
1:A:577:TRP:HA	1:A:580:ILE:HG22	1.86	0.57
3:B:1323:LEU:HD13	3:B:1436:VAL:HG21	1.87	0.57
1:A:340:LEU:C	1:A:340:LEU:HD23	2.30	0.57
1:A:41:ARG:HB3	1:A:43:GLN:HE21	1.69	0.56
3:B:1361:ASP:HB3	3:B:1435:LYS:HB2	1.87	0.56
1:A:299:MET:HE2	1:A:303:GLY:HA2	1.87	0.56
3:B:1368:PHE:HD1	3:B:1420:ILE:HG12	1.70	0.56
1:A:559:ASP:O	1:A:562:VAL:HG23	2.06	0.56
3:B:1255:ILE:HG22	3:B:1256:THR:N	2.21	0.55
2:G:857:ALA:O	3:B:1399:VAL:HG11	2.06	0.55
1:A:111:ASP:HB3	1:A:115:TYR:OH	2.07	0.55
2:G:818:VAL:HG13	2:G:820:GLU:H	1.73	0.54
3:B:1366:THR:CG2	3:B:1430:GLN:H	2.21	0.54
1:A:444:VAL:HG12	1:A:480:ASN:HA	1.90	0.54
1:A:128:MET:HE1	1:A:523:MET:HE1	1.90	0.53
2:G:787:ARG:NH2	2:G:789:MET:HE1	2.23	0.53
3:B:1480:HIS:CA	3:B:1481:GLN:CB	2.86	0.53
1:A:526:LEU:HD23	2:G:781:ALA:HB2	1.91	0.52
2:G:804:LYS:O	2:G:805:ASN:HB2	2.10	0.52
1:A:200:PRO:HD3	1:A:565:LEU:HD11	1.91	0.52
3:B:1323:LEU:HD13	3:B:1436:VAL:CG2	2.39	0.51
3:B:1344:LYS:HG2	3:B:1417:HIS:HB3	1.92	0.51
2:G:835:CYS:HB3	2:G:863:VAL:HB	1.91	0.51
1:A:89:PRO:O	1:A:90:GLN:HB2	2.09	0.51
1:A:342:VAL:HG11	1:A:357:VAL:HG21	1.92	0.50
2:G:825:ARG:CZ	2:G:845:ARG:NH1	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ALA:HA	1:A:368:THR:HG22	1.94	0.50
1:A:22:GLU:HG3	1:A:60:LEU:HD12	1.93	0.50
1:A:444:VAL:HG21	1:A:454:ILE:HD13	1.94	0.50
1:A:467:ILE:HD11	1:A:470:VAL:CG2	2.41	0.50
1:A:218:ASN:HB3	1:A:278:ARG:HH22	1.77	0.49
1:A:153:SER:O	1:A:154:ASN:ND2	2.45	0.49
3:B:1364:MET:HA	3:B:1364:MET:HE2	1.94	0.49
1:A:247:ILE:O	1:A:249:ASP:N	2.45	0.49
2:G:782:GLU:HG3	2:G:783:PRO:HD2	1.94	0.49
1:A:124:ARG:HG3	2:G:735:TRP:CZ2	2.48	0.49
1:A:388:PRO:HA	1:A:409:THR:HA	1.95	0.49
3:B:1366:THR:CG2	3:B:1429:ILE:HA	2.42	0.49
3:B:1392:ASP:O	3:B:1395:MET:HB2	2.13	0.49
2:G:861:VAL:HG12	3:B:1430:GLN:CD	2.38	0.49
3:B:1364:MET:HB2	3:B:1399:VAL:HG23	1.96	0.48
1:A:541:MET:HG3	2:G:758:LEU:HD21	1.95	0.48
1:A:475:ARG:NE	1:A:479:GLN:O	2.46	0.48
1:A:533:LEU:O	1:A:535:GLN:HG2	2.14	0.48
2:G:878:VAL:HG23	2:G:881:ALA:HB3	1.96	0.48
3:B:1362:ILE:HB	3:B:1401:VAL:HG13	1.94	0.48
1:A:247:ILE:HD12	1:A:252:LYS:HD2	1.96	0.47
1:A:588:THR:HG22	1:A:589:ALA:N	2.28	0.47
3:B:1368:PHE:CD1	3:B:1420:ILE:HG12	2.48	0.47
2:G:720:ASP:OD2	2:G:720:ASP:C	2.57	0.47
2:G:816:ASN:OD1	2:G:818:VAL:HG12	2.14	0.47
3:B:1506:LEU:HD22	3:B:1553:LEU:HB3	1.96	0.47
1:A:61:VAL:HG12	1:A:63:PRO:HD3	1.97	0.47
1:A:233:GLU:HG3	1:A:234:GLU:N	2.30	0.47
1:A:607:THR:HG23	1:A:613:ASN:OD1	2.14	0.47
2:G:720:ASP:HA	2:G:723:ILE:HD12	1.96	0.47
1:A:41:ARG:HB3	1:A:43:GLN:NE2	2.30	0.47
3:B:1258:GLU:HB2	3:B:1290:THR:HB	1.97	0.47
3:B:1487:PRO:O	3:B:1490:ILE:HG12	2.14	0.46
1:A:206:LEU:HD11	1:A:296:VAL:HG11	1.97	0.46
2:G:814:LEU:HD11	2:G:826:VAL:HG21	1.98	0.46
3:B:1506:LEU:HD23	3:B:1554:LYS:C	2.41	0.46
1:A:153:SER:O	1:A:154:ASN:CB	2.63	0.46
3:B:1507:LEU:HD11	3:B:1521:ASP:HB2	1.96	0.46
2:G:742:GLU:OE2	2:G:752:LYS:HG2	2.16	0.46
2:G:924:LYS:HA	3:B:1288:ASP:HB3	1.98	0.46
1:A:66:GLU:O	1:A:68:PRO:HD3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:O	1:A:467:ILE:CG2	2.64	0.46
1:A:215:ILE:HG13	1:A:317:VAL:O	2.16	0.46
1:A:529:LYS:HD2	1:A:546:GLU:OE1	2.16	0.45
3:B:1506:LEU:HD23	3:B:1554:LYS:O	2.17	0.45
3:B:1596:GLU:HG3	3:B:1598:GLU:H	1.81	0.45
2:G:908:LEU:HD23	3:B:1300:THR:HB	1.98	0.45
2:G:939:THR:HA	3:B:1304:LEU:O	2.16	0.45
3:B:1322:HIS:O	3:B:1347:THR:HA	2.17	0.45
3:B:1490:ILE:HG13	3:B:1491:GLU:N	2.31	0.45
1:A:426:ALA:HB3	1:A:441:ASN:HB2	1.98	0.45
1:A:332:PHE:CD2	1:A:380:ILE:HD12	2.53	0.44
3:B:1542:ILE:HB	3:B:1578:ILE:HG22	1.98	0.44
1:A:68:PRO:HB2	1:A:70:LYS:HE2	1.99	0.44
1:A:146:PRO:HD3	1:A:175:TRP:CD1	2.51	0.44
2:G:782:GLU:HG3	2:G:783:PRO:CD	2.47	0.44
2:G:926:ARG:HH11	3:B:1303:ILE:HG21	1.81	0.44
3:B:1547:CYS:O	3:B:1551:LEU:HD12	2.17	0.44
1:A:355:VAL:H	1:A:368:THR:HB	1.82	0.44
1:A:450:SER:O	1:A:453:GLN:HB2	2.18	0.44
1:A:111:ASP:HB2	1:A:122:LEU:HB2	2.00	0.44
1:A:467:ILE:HD11	1:A:470:VAL:HG22	1.99	0.44
3:B:1255:ILE:CG2	3:B:1256:THR:N	2.81	0.44
1:A:429:SER:HB2	1:A:438:LEU:HD13	2.00	0.43
1:A:105:PHE:CZ	1:A:580:ILE:HG12	2.52	0.43
1:A:537:PRO:HB3	2:G:760:ASP:HA	1.99	0.43
3:B:1482:GLU:O	3:B:1602:LEU:CD1	2.64	0.43
3:B:1358:THR:HA	3:B:1438:SER:HA	2.01	0.43
1:A:26:ASP:OD2	1:A:30:LYS:NZ	2.50	0.43
1:A:368:THR:HG23	1:A:372:GLY:HA2	2.01	0.43
3:B:1484:ILE:HB	3:B:1605:ASP:HB3	2.00	0.43
1:A:577:TRP:HE3	1:A:580:ILE:HG21	1.84	0.43
3:B:1341:LEU:HB2	3:B:1420:ILE:HG23	2.00	0.43
2:G:824:VAL:O	2:G:847:GLN:HA	2.19	0.43
3:B:1256:THR:HG23	3:B:1292:THR:HB	2.01	0.43
3:B:1469:ARG:HD2	3:B:1568:LEU:O	2.18	0.43
3:B:1349:TYR:CE2	3:B:1351:GLY:HA3	2.54	0.43
1:A:238:VAL:HG21	3:B:1404:TYR:CE1	2.54	0.42
1:A:526:LEU:HD13	2:G:771:SER:HB3	2.00	0.42
1:A:89:PRO:O	1:A:90:GLN:CB	2.66	0.42
1:A:206:LEU:HD11	1:A:296:VAL:CG1	2.48	0.42
1:A:443:ASN:OD1	1:A:481:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:HG23	1:A:149:ILE:O	2.19	0.42
1:A:231:TYR:HB2	2:G:789:MET:HG3	2.01	0.42
3:B:1562:TRP:CD1	3:B:1562:TRP:C	2.97	0.42
1:A:197:TYR:HE1	1:A:199:LEU:CD1	2.32	0.42
1:A:543:ILE:HG12	2:G:756:PHE:HE2	1.83	0.42
3:B:1369:LEU:HA	3:B:1370:PRO:HD3	1.91	0.42
1:A:170:VAL:HG22	1:A:175:TRP:HZ2	1.85	0.42
1:A:426:ALA:C	1:A:427:ILE:HD12	2.45	0.42
1:A:519:LYS:HA	5:A:668:HOH:O	2.20	0.42
2:G:903:VAL:HG22	3:B:1304:LEU:HD23	2.02	0.41
2:G:825:ARG:O	2:G:876:ALA:HA	2.20	0.41
1:A:34:ILE:HB	1:A:86:VAL:HG12	2.01	0.41
1:A:111:ASP:OD1	1:A:112:LYS:HG2	2.20	0.41
1:A:416:GLN:NE2	1:A:508:GLU:HA	2.35	0.41
1:A:588:THR:HB	5:A:670:HOH:O	2.20	0.41
1:A:563:TYR:N	1:A:563:TYR:CD2	2.88	0.41
3:B:1531:ASP:HB2	3:B:1565:ARG:NH2	2.35	0.41
1:A:142:GLU:HG2	1:A:153:SER:HB2	2.03	0.41
1:A:365:MET:HE2	1:A:365:MET:HB3	1.74	0.41
2:G:802:VAL:HG12	2:G:803:VAL:N	2.34	0.41
3:B:1306:PHE:CD1	3:B:1306:PHE:N	2.88	0.41
3:B:1500:TYR:O	3:B:1562:TRP:HB2	2.21	0.41
3:B:1512:GLN:O	3:B:1513:ASP:C	2.63	0.41
1:A:588:THR:CG2	5:A:667:HOH:O	2.67	0.41
3:B:1366:THR:HG22	3:B:1430:GLN:N	2.32	0.41
2:G:798:MET:HE3	2:G:810:ILE:CG2	2.44	0.41
1:A:577:TRP:HA	1:A:580:ILE:CG2	2.50	0.41
2:G:787:ARG:NH2	2:G:789:MET:CE	2.83	0.40
1:A:247:ILE:HG12	1:A:290:HIS:CE1	2.57	0.40
2:G:816:ASN:HB2	2:G:822:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	594/627 (95%)	562 (95%)	29 (5%)	3 (0%)	24	44
2	G	209/252 (83%)	194 (93%)	15 (7%)	0	100	100
3	B	333/379 (88%)	298 (90%)	26 (8%)	9 (3%)	4	6
All	All	1136/1258 (90%)	1054 (93%)	70 (6%)	12 (1%)	11	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	ASP
3	B	1533	ASN
3	B	1428	PHE
3	B	1473	GLU
3	B	1481	GLN
3	B	1572	LYS
3	B	1261	ASP
1	A	154	ASN
3	B	1496	THR
1	A	258	LEU
3	B	1466	ASN
3	B	1534	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	521/548 (95%)	495 (95%)	26 (5%)	22	44
2	G	191/227 (84%)	169 (88%)	22 (12%)	5	10
3	B	289/345 (84%)	268 (93%)	21 (7%)	13	27
All	All	1001/1120 (89%)	932 (93%)	69 (7%)	14	30

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	44	LYS
1	A	60	LEU
1	A	79	ASN
1	A	94	GLU
1	A	176	ARG
1	A	198	VAL
1	A	199	LEU
1	A	218	ASN
1	A	292	LEU
1	A	328	THR
1	A	340	LEU
1	A	341	THR
1	A	368	THR
1	A	378	LEU
1	A	382	LEU
1	A	400	ARG
1	A	415	THR
1	A	481	LEU
1	A	483	THR
1	A	499	VAL
1	A	533	LEU
1	A	562	VAL
1	A	570	LYS
1	A	580	ILE
1	A	596	LEU
2	G	720	ASP
2	G	723	ILE
2	G	737	THR
2	G	743	GLU
2	G	752	LYS
2	G	753	THR
2	G	755	SER
2	G	778	ILE
2	G	782	GLU
2	G	798	MET
2	G	813	ILE
2	G	816	ASN
2	G	818	VAL
2	G	827	GLU
2	G	842	GLN
2	G	845	ARG
2	G	862	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	898	VAL
2	G	906	VAL
2	G	920	LEU
2	G	921	GLU
2	G	937	ILE
3	B	1256	THR
3	B	1300	THR
3	B	1310	GLN
3	B	1344	LYS
3	B	1356	THR
3	B	1358	THR
3	B	1390	GLU
3	B	1392	ASP
3	B	1401	VAL
3	B	1421	LEU
3	B	1441	ASN
3	B	1462	ILE
3	B	1474	THR
3	B	1484	ILE
3	B	1509	ILE
3	B	1530	THR
3	B	1580	THR
3	B	1593	GLU
3	B	1596	GLU
3	B	1600	GLN
3	B	1615	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	154	ASN
1	A	165	ASN
1	A	311	GLN
1	A	346	ASN
1	A	414	GLN
2	G	846	GLN
2	G	867	GLN
2	G	944	GLN
3	B	1322	HIS
3	B	1397	GLN
3	B	1417	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1480	HIS
3	B	1539	HIS
3	B	1600	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	602/627 (96%)	0.05	11 (1%) 67 63	36, 50, 67, 76	0
2	G	215/252 (85%)	0.49	20 (9%) 14 11	40, 56, 90, 98	0
3	B	343/379 (90%)	0.65	29 (8%) 16 13	41, 67, 87, 91	0
All	All	1160/1258 (92%)	0.31	60 (5%) 33 27	36, 55, 83, 98	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	564	VAL	5.1
2	G	910	PRO	4.0
2	G	905	ILE	3.8
3	B	1513	ASP	3.8
3	B	1515	ASN	3.4
3	B	1424	PHE	3.3
3	B	1530	THR	3.3
2	G	909	ASP	3.2
3	B	1283	THR	3.2
1	A	623	PRO	3.1
3	B	1291	VAL	3.0
1	A	565	LEU	2.9
2	G	940	LYS	2.9
2	G	903	VAL	2.9
3	B	1257	ILE	2.8
3	B	1251	LEU	2.8
2	G	904	THR	2.8
3	B	1514	GLY	2.8
2	G	907	LYS	2.7
2	G	943	ILE	2.7
2	G	898	VAL	2.7
3	B	1266	ILE	2.6
3	B	1256	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	942	ILE	2.6
2	G	935	THR	2.5
3	B	1382	VAL	2.5
1	A	79	ASN	2.5
2	G	791	VAL	2.5
3	B	1512	GLN	2.4
2	G	902	ILE	2.4
3	B	1303	ILE	2.4
2	G	908	LEU	2.4
3	B	1281	VAL	2.4
3	B	1585	ILE	2.3
3	B	1531	ASP	2.3
2	G	944	GLN	2.3
2	G	922	VAL	2.3
3	B	1299	ALA	2.3
2	G	882	LEU	2.3
1	A	186	GLU	2.3
1	A	70	LYS	2.3
2	G	843	ARG	2.3
3	B	1511	GLU	2.2
1	A	536	MET	2.2
1	A	185	PRO	2.2
3	B	1573	ASP	2.2
1	A	383	ASN	2.2
2	G	920	LEU	2.1
1	A	151	VAL	2.1
2	G	923	ILE	2.1
3	B	1581	LYS	2.1
3	B	1265	PRO	2.1
3	B	1255	ILE	2.1
1	A	563	TYR	2.0
3	B	1388	ARG	2.0
3	B	1473	GLU	2.0
3	B	1280	THR	2.0
3	B	1580	THR	2.0
3	B	1253	LEU	2.0
3	B	1285	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	A	628	1/1	0.98	0.04	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.